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Application of an optimization tool for inverse modelling of thin-film silicon solar cells

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Abstract

Device simulation of thin-film silicon solar cells depends strongly on good input parameters, but many of the electronic parameters are difficult to determine by experiment. Therefore inverse modelling, i.e., the determination of simulation input parameters by adjusting simulation results to given experimental data, is very useful. We have developed a systematic procedure of inverse modelling with makes use of a particle swarm optimization algorithm. Experimentally determined external quantum efficiency, dark and illuminated current-voltage characteristics were modelled to determine the input parameters, resulting in very good agreement between the simulation and experiment.

Keywords: inverse modelling; amorphous silicon; microcrystalline silicon; particle swarm optimization; solar cell; device simulation; quantum efficiency; current-voltage characteristics

1. Introduction

Simulations of thin-film silicon solar cells are usually based on the numerical solution of Poisson's equation and the continuity equations with appropriate expressions for the currents. The result of these

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simulations depends very much on the optical and electrical input parameters for which a proper choice is thus very important. Some of the input parameters can be measured experimentally. Some other input parameters can hardly or not at all be measured, e.g., capture cross sections of defects and distribution of the trap states in the band gap. Here inverse simulation is a very useful technique. While in forward modelling, input parameters (such as band gap, defect properties) are given and the behaviour of the device is calculated (e.g. the current-voltage characteristic or the quantum efficiency), inverse modelling goes just the other way round. Here the desired output is given, usually by experiment, and the input parameters that lead to comparable simulation results are determined. A huge amount of simulations are performed in order to determine the set of input parameters that fits best to the desired device behaviour. Optimization algorithms are used for sophisticated choices of input parameters. A set of input parameters that describes one measurement can be found by hand, but describing several different measurements properly is difficult.

Inverse modelling was applied to semiconductor device simulation by Owerling to determine a doping profile [1]. In his optimization tool 'Profile' the 'Modified Damped Last Squares' method is implemented. This optimization tool was also used by Zeman and Willemen to calibrate solar cell simulations [2,3].

In this paper we show that the particle swarm algorithm [4,5] is a suitable optimization algorithm to perform inverse modelling on the basis of the current voltage (*IV*) characteristics (illuminated and dark) and the external quantum efficiency (EQE). For demonstration, we model both a hydrogenated amorphous silicon (a-Si:H) and a hydrogenated microcrystalline (μc-Si:H) single *pin* junction solar cell.

2. Experimental

A 0.6 cm^2 a-Si:H single junction cell and a μc-Si:H single junction cell of the same size were used to measure illuminated and dark *IV*-characteristics and EQE. The silver back contact defines the cell size. For the illuminated *IV*-curve a mask, slightly smaller than the cell size, was used to illuminate a defined area with the AM1.5 spectrum. The EQE was measured with AM1.5 bias. Optical data were measured by ellipsometry measurements for every layer of the *pin* solar cells, deposited directly on glass. As no single layer μc-Si:H samples were available optical data from related μc-Si:H films were used.

3. Inverse Modelling with optiSLang

The result of the procedure of inverse modelling strongly depends on the used optimization algorithm. The particle swarm optimization (PSO), used here, imitates the behaviour of a swarm of animals searching for food in a landscape. Each animal of the swarm corresponds to one design (=one set of input parameter values). The landscape is the design variable space, and the desirable position is the one where the objective function or functions (here the error between simulation and experiment) are minimized. As result the Pareto front is determined. A design is part of the Pareto front if there is no other design that is better in all objectives. More details of the working principle of the PSO with only one objective can be found in [4] or for several objectives in [5].

We used inverse modelling to determine electrical input parameters for simulations of a-Si:H and μc-Si:H single junction solar cells that lead to simulation results that fit the experimental data.

The particle swarm algorithm of the commercially available tool optiSLang [6] was applied as optimization tool and ASA [7] as device simulator. In Fig.1 the procedure of inverse modelling is sketched. The PSO produces a first set of input parameters randomly and passes them to ASA. The error between the simulation and measurement is determined by calculating the mean square deviation for the illuminated *IV*, EQE and logarithmic dark *IV*. The PSO determines the next generation designs taking the results of the previous generations of all or at least several of the particles into account.

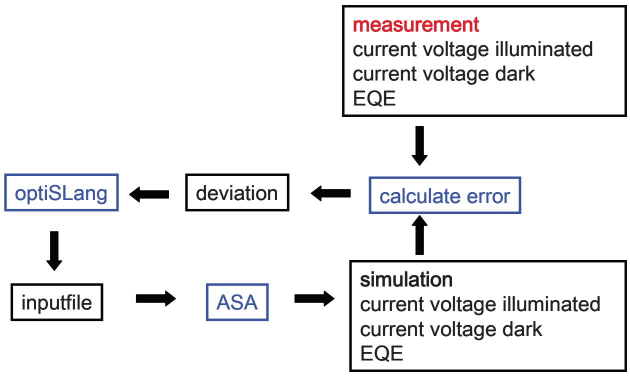

Fig.1: The procedure of inverse modelling applied: optiSLang produces many different input parameter sets and passes them to ASA. The simulation result of every input parameter set is compared with the experimental measurement for EQE, illuminated and dark *IV*-characteristics. The calculated error is passed to optiSLang. Here it is taken into account for the parameters of the next generation.

In our case there are three objectives for a-Si:H the error of the illuminated *IV*-characteristics, the error of the dark *IV*-characteristics and error of the EQE. We used only two objectives for the µc-Si:H cell, namely the illuminated and dark *IV*-characteristic. The EQE of µc-Si:H is not used in the optimization procedure, as the optical data have the major influence here and were not known precisely.

4. Results and Discussion

The input parameters for an a-Si:H single junction and a µc-Si:H single junction cell were determined by the procedure described above. In both cases a parameter set was found that can describe illuminated and dark *IV*-characteristics very well, see Figs. 2 and 3. For the inverse modelling data points of the dark (illuminated) *IV*-characteristics from 0.5 V to 2.3 V (0 V to 0.9 V) were used for the a-Si:H and from 0.17 V to 2.3 V (-0.5 V to 0.7 V) for µc-Si:H cell. The dark *IV*-characteristic is shown in logarithmic and linear scale in Fig. 2. Fig. 2(a) illustrates that the parallel resistance dominates the *IV*-characteristic of the a-Si:H cell below 0.5 V. Therefore the value of the parallel resistance can be determined easily by hand. The dark current density of the µc-Si:H cell is very high so that we see almost no influence of the parallel resistance. The range of high voltages is strongly influenced by the series resistance, but also by the mobility. Therefore we determine both series resistance and mobility with inverse modelling.

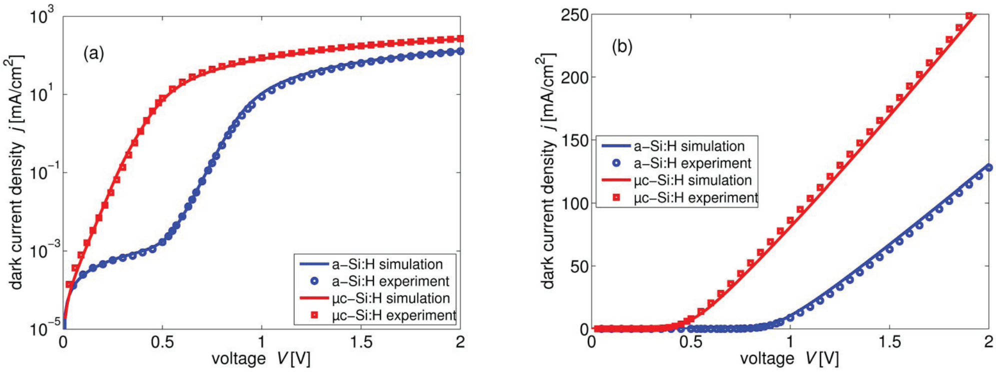

Fig. 2: The experimental and simulated dark *IV*-characteristics of the a-Si:H and µc-Si:H single junction solar cell in (a) logarithmic and (b) linear scale. The full lines show the simulation results, determined by inverse modelling. Three objectives (EQE, *IV* illuminated and *IV* dark) were used for a-Si:H and two objectives (*IV* illuminated and *IV* dark) for µc-Si:H.

With the parameters determined by inverse modelling good agreement between the experimental and simulated illuminated *IV*-characteristics, for a-Si:H and μc-Si:H, is achieved, see Fig. 3(a). For the a-Si:H single junction solar cell the EQE is also described well in Fig. 3(b). The deviations in the EQE of μc-Si:H cell between experiment and simulation are due to poor optical data. Usually we determine the optical data by ellipsometry measurements on single layers deposited on glass. Due to the lack of proper μc-Si:H thin-films on glass, the optical data were determined from μc-Si layers produced in a different setup. Nevertheless, the integrated EQE fits well to the short-circuit current density, so that the simulation of the illuminated *IV*-characteristics can be done without any correction factor for the generation profile.

The parameters we determined by inverse modelling for the a-Si:H cell are: hole mobility, electron mobility, distance between Fermi level and conduction band edge in n-a-Si, distance between Fermi level and valence band edge in p-a-Si, slope of valence band tail in i-a-Si and p-a-Si, slope of conduction band tail in i-a-Si, series resistance and peak position of the Gaussian defect pool. Electron mobility, hole mobility and the peak position of the Gaussian defect pool are equal for all layers (p-a-Si, i-a-Si, n-a-Si). For the other parameters values employed in the literature [2,8,9,10] were used. For the μc-Si:H cell far more parameters (~30) were optimized to reach the results shown in Fig.2 and Fig.3.

The good agreement in Figs. 2 and 3 between the experimental and simulated data illustrates that the PSO algorithm successfully works with several objectives.

The question weather it is possible to find a unique set of parameters for the simulated data in Figs. 2 and 3 was addressed as well. Therefore several optimization runs for a-Si:H with different parameters to be determined by the optimization were performed. In these optimizations we did not take the EQE as objective into account because it is quite difficult to decide weather a unique solution is reached when having more than two objectives because of the visualization of the 3d Pareto-front.

In fact the optimization has many solutions as all Pareto optimal solutions are equally good results from optiSLang's point of view. As the Pareto front contains designs that may have a large error in one objective it is not useful to focus on the Pareto front as a whole for finding acceptable solutions. In fact, only a small portion of the Pareto front is suitable in which the solutions have small enough errors for all the objectives. This limited number of designs may then inspected by eye. Still there are several designs that give equally good results. To find out weather we have a unique solution we have to check if these parameter sets are similar to each other or not. It depends on the parameters that we determined by inverse modelling if we find no solution, a unique solution or a lot of solutions.

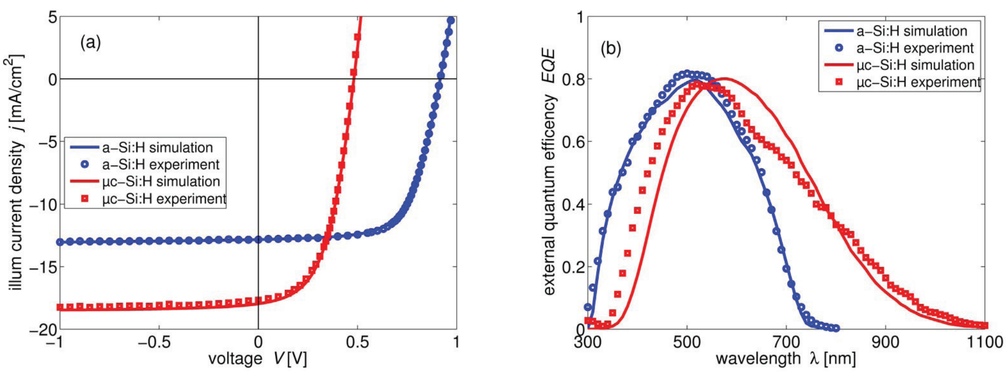

Fig. 3: The illuminated *IV*-characteristics (a) and the EQE (b) of the a-Si:H and μc-Si:H single junction solar cells are simulated with same input parameters as the corresponding dark *IV*-characteristics of Fig. 2. The optical data used in the measurement were determined by ellipsometry measurements.

When searching for all input parameters that are available at the same time it is not possible to find a unique solution. This is in agreement with the result of Willemen [2]. As the time needed for one inverse modelling run rises with the number of input parameters that have to be determined it is favourable to optimize as few as possible.

Our investigation indicates that using seven parameters (hole mobility, electron mobility, distance between Fermi level and conduction band edge, distance between Fermi level and valence band edge, slope of valence band tail, slope of conduction band tail and series resistance), a unique solution can be found for a-Si:H. Of course the result depends on the values of the other input parameters that were fixed during the simulation. In any case, the optimization works better when it has a unique solution.

When using less non-fixed parameters we cannot get a good solution when the fixed input parameters do not already have optimized values.

5. Conclusions

The combination of the device simulator ASA and the particle swarm optimizer of the software optiSLang is demonstrated to be very appropriate to determine a set of parameters that describes illuminated and dark *IV*-characteristics of thin-film silicon solar cells very well. Finding a unique solution depends on the number of input parameters that are to be found by inverse modelling and on the number of measurements that can be used for comparison.

This method to perform inverse modelling was established successfully. In further work this procedure will be performed with better optical data. Measurements on cells with intrinsic-layer thickness variations will be used for validation to find reliable parameters for our cells.

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